Open-Ended Problems: A Future Chemical Engineering Education Approach. J. Patrick Abulencia and Louis Theodore.

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Term Projects (2): Chemical Reactors

Term Project 29.1

Minimizing Volume Requirements for CSTRs in Series I

CSTRs in series are usually designed so that the volumes of the individual reactors are equal. For almost all reactions, the total volume requirement for achieving a given conversion decreases as the number of reactors in series increases. This can significantly impact the economics, particularly the capital cost. However, the total volume requirement to achieve a particular conversion can be further reduced, particularly for non-elementary reactions, if the constraint of equal reactor volumes is removed, i.e., the volumes of each reactor need not be the same. Although these systems can be designed to lower volume requirements, the impact on the overall economics can be negative [1,2].

Consider the elementary irreversible reactions between

$$A + B \rightarrow \text{products} \tag{29.1}$$

If one employs a feed containing equimolar concentrations of reactants, the reaction rate expression can be written as

$$-r_A = k_A C_A C_B = kC_A^2; \quad k = k_A \tag{29.2}$$

One can calculate the reactor size requirements for either one CSTR or for a cascade composed of n identical CSTRs. Assume isothermal operation at 25°C where the reaction rate constant is equal to 9.92 $m^3/(kgmol \cdot min)$. Reactant concentrations in the feed are each equal to 0.08 $kgmol/m^3$, and the liquid feed rate is equal to 0.278 m^3/min. The desired degree of conversion is 87.5% [3].

Outline a procedure to calculate the volume requirement of a cascade of n CSTRs, that *differ* in size for the *minimum* total volume and the manner in which the total volume should be distributed between the n reactors.

Also use the equation(s) developed for n reactors to calculate the minimum volume requirement for three different n values of your choice, e.g., 2, 5, and 7. Comment on the results.

Term Project 29.2

Minimizing Volume Requirements for CSTRs in Series II

Refer to the previous term project concerned with CSTRs in series. *Outline* how to solve the problem if the rate of reaction is once again given as

$$-r_A = k_A C_A C_B = kC_A^2; \quad k = k_A \tag{29.3}$$

but with the variation of k_A with temperature dictated by the Arrhenius equation, i.e.,

$$k = Ae^{-E/RT} \tag{29.4}$$

Assign an enthalpy of reaction (assume it to be exothermic) with the Arrhenius equations coefficients given by A and E for the reaction under consideration and redesign the *n*-stage CSTR system taking enthalpy of reaction effects into account. Assume the enthalpy of reaction is constant (and independent of temperature) and the operation is adiabatic. This effectively means that the temperature in the *n* reactors will *not* be 25°C. Once again, the *n* CSTRs will differ in size in order to satisfy the *minimum* total volume requirement [4,6].

After the solution has been outlined, assign at least three sets of values to A and E; i.e.,

$$\begin{array}{l} A_1, E_1 \\ A_2, E_2 \\ A_3, E_3 \\ \;.\quad . \\ \;.\quad . \end{array} \tag{29.5}$$

and solve the problem. The A and E values should be such that one can provide a meaningful analysis of the effect of A and E on the results.

References

1. L. Theodore, *Chemical Reaction Kinetics*, A Theodore Tutorial, Theodore Tutorials, East Williston, NY, originally published by the USEPA/APTI, RTP, NC, 1992.

2. L. Theodore, *Chemical Reactor Analysis and Applications for the Practicing Engineer*, John Wiley & Sons, Hoboken, NJ, 2012.
3. Adapted from: J. Reynolds, J. Jeris, and L. Theodore, *Handbook of Chemical and Environmental Engineering Calculations*, John Wiley & Sons, Hoboken, NJ, 2004.
4. L. Theodore, *Chemical Reaction Kinetics*, A Theodore Tutorial, Theodore Tutorials, East Williston, NY, originally published by the USEPA/APTI, RTP, NC, 1992.
5. L. Theodore, *Chemical Reactor Analysis and Applications for the Practicing Engineer*, John Wiley & Sons, Hoboken, NJ, 2012.
6. Adapted from: J. Reynolds, J. Jeris, and L. Theodore, *Handbook of Chemical and Environmental Engineering Calculation*s, John Wiley & Sons, Hoboken, NJ, 2004.